PORTLAND HARBOR RI/FS

REMEDIAL INVESTIGATION REPORT

# APPENDIX A3
# SCRA DATABASE AND DATA MANAGEMENT

**(SCRA Database Provided ~~on Accompanying CD~~in Separate File)**

**DRAFT FINAL**

June 12, 2015

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# 1.0 INTRODUCTION

This appendix presents the site characterization and risk assessment (SCRA) database and the data ~~management rules~~usability issues, quality assurance/quality control checks, ~~used to~~and the selection criteria for~~ reduce the SCRA data set into~~ the remedial investigation (RI), baseline human health risk assessment (BHHRA), and baseline ecological risk assessment (BERA) data sets. A brief discussion of the U.S. Environmental Protection Agency's (USEPA) Query Manager™ is also provided.~~ data set used to present information in Sections 5.0 of the RI Report. Further reduction and refinement of the SCRA data set was developed and completed by Kennedy/Jenks (Appendix F) and Windward Environmental (Appendix G) for risk analyses. This further refinement is not discussed here. The data management rules (including data reduction, data usability, and data quality) used to develop the RI data set are described in Section 2.0 of the RI Report.~~

Commented [A1]: Integral:

The redline text is information previously provided in Section 2 and is included here because it is important information regarding the RI database.

## 1.1 DATA USABILITY

As discussed in Section 2.2 of the RI, the principal issues related to the usability of historical and current data include data quality, sediment stability over time, and the intended use of the data. All of these factors must be acceptable for data to be considered usable. This section describes some of the more commonly encountered, and perhaps most consequential, data usability issues for the Portland Harbor Remedial Investigation and Feasibility Study (RI/FS)—elevated detection limits for non-detected chemical concentration data and N-qualified chemical concentration data.

### 1.1.1 Elevated Detection Limits

The historical database for Portland Harbor contains some samples with non-detected concentrations of constituents at high detection limits. From a purely analytical perspective, USEPA categorizes all data meeting proper quality assurance and quality control (QA/QC) procedures, regardless of detection limit level, as Category 1 (i.e., data of known quality and considered acceptable for use). However, the acceptability of these data is dependent on their specific use. For example, in the absence of other data, elevated detections limits may provide insight on the need for additional analyses for which lower detection limits are achievable. From a data-needs standpoint, however, these same data may not be useful because if inappropriately compared to a concentration benchmark, they could unnecessarily result in the perceived need for additional sampling and analysis (despite their attendant uncertainty in actual concentration). From a predictive risk assessment perspective, these data are recommended by USEPA to be excluded from formal risk quantification because of their uncertainty in concentration (USEPA 1989). From an applied engineering and feasibility standpoint, elevated detections limits are also not useful because they are not capable of defining with precision actual chemical concentration data that can be used to set boundaries for remedy considerations.

### 1.1.2 N-qualifiers

N-qualified data present another situation that requires evaluation in the context of data use. N-qualified data in the RI data set are identified and used in the RI and risk assessments with recognition of the potential limitations associated with using this data noted below.[1] The N-qualifier denotes that the identity of the analyte is presumptive and not definitive, generally as a result of the presence in the sample of an analytical interference, such as hydrocarbons or, in the case of pesticides, polychlorinated biphenyls (PCBs). Data that are N-qualified meet the primary identification criteria of the method; however, the confirmation criteria are not met and the identification is potentially a false positive. In addition to uncertainty regarding chemical identification, N-qualified data also indicate some uncertainty in the reported concentration level (USEPA 1989). The degree of attendant uncertainty in both identification and concentration is commonly assessed on a sample-by-sample basis.

Given the uncertainty associated with N-qualified data, as well as the varying extent of this uncertainty, users must carefully weigh the impacts of their use throughout the RI/FS process. This careful attention is fully consistent with USEPA guidance and other data-use guidance documents recommending the use of N-qualified data only on a case-by-case basis. The rationale for this is that data are evaluated and used in different ways throughout the RI/FS process. Provided below are some examples of how intended use of N-qualified data could vary:

- **Nature and Extent.** In nature and extent determinations, evaluations of data are generally predicated on individual, point-by-point analytical results (e.g., determining the individual chemical concentration results at various sample locations as opposed to calculating a mean across those samples). In instances when N-qualified data are spatially accompanied by data of more certain chemical identification and concentration, the role of N-qualified data is likely limited. This is often the case for Portland Harbor, where there exists an abundance and wide distribution of data for sediment, surface water, and biota that are not N-qualified. The number and percentage of N-qualified data for the nature and extent indicator contaminants (see RI Section 5.0) for all media are summarized in Table A3-1 and details are provided in data reports and site characterization summary reports for the various sampling tasks.

- **Risk Assessment.** N-qualified data are present in the database, and USEPA requested that these data be included in the risk assessments. USEPA (1989) recognizes that while uncertainty in both chemical identity and chemical concentration exists for N-qualified data, their use in risk assessment is judged on a case-by-case basis. N qualification indicates “the presence of an analyte that has been ‘tentatively identified,’ and the associated numerical value

[1] Consistent with Risk Assessment Guidance for Superfund Part A (USEPA 1989), N-qualified data were included in the data set used for risk assessment, as documented here.

represents its approximate concentration" (USEPA 1999). The qualification indicates that the analyst believed that the result was caused by analytical interference from a chemical other than the target analyte. All N-qualified results are therefore biased high for organochlorine pesticides and may result in an overestimation of risk.

## 2.0 SCRA DATABASE

Integral's LWG project database contains all of the data reported by the analytical laboratories. This includes field and lab replicates, lab dilutions, results for the same analyte from multiple analytical methods (SW8270 and SW8270-SIM, for example), and laboratory QA samples such as matrix spikes, surrogates, and method blanks. The data handling rules described in *Guidelines for Data Averaging and Treatment of Non-detected Values for the Round 1 Database* (Kennedy/Jenks et al. 2004) were used to create a data set for the SCRA data users that was simpler; the data set contained only one result per analyte per sample and excluded all of the laboratory QA results. This involved creating a SCRA database that excluded lab QA results, contained only the most appropriate dilution result and analytical method for each analyte, and contained the average of laboratory replicates. For purposes of reporting, both LWG data and data collected by other parties were combined into one SCRA database. Guidelines provided in Kennedy/Jenks et al. (2004) were consistently applied to all data sets. The resulting SCRA database is provided on a CD accompanying this appendix~~.~~, and reflects a data lockdown date of July 19, 2010.

~~The SCRA database included here reflects a data lockdown date of June 2, 2008. As part of the revision process, a new database lockdown date of July 19, 2010 was established to incorporate data sets collected since June 2008. The updated SCRA database is provided in Appendix H.~~

## 3.0 DATA MANAGEMENT QA/QC

~~Quality assurance/quality control (~~QA/QC~~)~~ checks were made throughout the LWG's data management process. The data management team, composed of database managers and chemists, performed checks of accuracy and completeness in two separate databases. Analytical data are stored in EQuIS™, a relational Microsoft Access™-based software system. Each participating laboratory sent data in EQuIS-compatible electronic data deliverables (EDDs) to both the database manager and the data validator. Checks began at that point, as listed in the table below, and again later when the database manager updated the database with the validator's revised EDD. At the same time, a sample tracking database developed in Access monitored data flow and sample analytical completeness. Data collected by other parties was ~~either~~ received either in hardcopy or in electronic format. Because some data were hand-entered, a percentage of the results was verified by a second staff member. If errors were found, 100 percent of the data in the data set was checked.

In developing the SCRA, redundant checks were made on much of the same data checked in the EDDs. Other specific checks are as follows:

- **Completeness**—Chain-of-custody forms submitted to the laboratory listing samples, methods, and analyses were compared to samples, methods, and analytes loaded into the SCRA for each sampling event. These checks were made for all samples. For data sets prepared by other parties, the source document was typically used to check sample/method/analyte completeness in the SCRA.
- **Averaging**—Laboratory duplicates and field splits were averaged. Because averaging required significant data manipulation, a series of additional checks were performed on the SCRA database before distribution. Data were divided into subgroups, and approximately 40 percent of the data in each subgroup was verified. If any problems were found with the averaging, then 100 percent of the data in the subgroup was verified, and problems were corrected.
- **Database Codes**—Project database codes were checked for sample type, matrix type, basis, and units. Unusually high and low values for a given method were checked to confirm potential unit or analytical errors.
- **Qualifiers**—Checks were made for unusual data qualifier codes. Qualifier codes for calculated averages followed guidelines provided in Kennedy/Jenks et al. (2004) and are listed below. ("A" and "T" are considered descriptors rather than qualifiers):

| Qualifier/Descriptor | Description |
|---|---|
| A | Summed value based on limited number of analytes. |
| J | Estimated value. |
| JA | Combined qualifier. |
| JT | Combined qualifier. |
| N | Presumptive evidence of a compound. |
| NJ | Combined qualifier. |
| NJT | Combined qualifier. |
| NT | Combined qualifier. |
| R | Rejected. |
| T | Result derived or selected from >1 reported value. |
| U | Analyte was analyzed for but not detected. |
| UA | Combined qualifier. |
| UJ | Not detected. Sample detection limit is estimated. |
| UJA | Combined qualifier. |

In addition to the standard checks above, Integral Consulting Inc.'s (Integral) senior chemists reviewed all final SCRA files prior to distribution. QA/QC checks for each major step are provided in the table below.

### LWG-Generated Data Quality Checks

| Data Management Step | QA/QC Step |
|---|---|
| Receive EDD from lab | Check samples: correct type (normal, replicate, blank, etc.), correct matrix, correct task |
| | Check tests: expected methods, correct lab matrix, correct basis |
| | Check results: correct analyte codes, correct result type (target, surrogate, spiked compound, etc.), detection limits reported |
| Load lab EDD | Check samples match with tests, tests match with results |
| Receive EDD from validator | Check lab and validator qualifiers are propagated to final qualifier |
| | Check reason code is assigned for all validator qualifiers |
| | Check that detection limit is updated for results restated as non-detects |
| Load validator EDD | Check that validated results exactly match with existing sample/method/date/time/analyte, and if not, verify they should be changed |
| SCRA data reduction[*a] | Check for sample/method/analyte completeness |
| | Check again for correct sample type, matrix, basis, and units |
| | Check for unusually high/low values |
| | Check for unusual qualifiers |

[*a] Performed by Senior Information Manager

### LWG Sample Tracking Database

| Sample Tracking Step | QA/QC Step |
|---|---|
| Enter sample information from ~~FSP~~field sampling plan | Check entries 100% |
| Receive sample confirmation from lab~~,~~ enter samples and associated analytical groups | Check entries 100%; compare ~~FSP~~ field sampling plan list with sample confirmation list |
| Receive lab EDDs~~,~~ enter sample, sample delivery group, and analytical group information | Check analytical completeness and lab progress on a weekly basis during sampling events |

### Quality Checks for Data Collected by Other Parties

| Data Management Step | QA/QC Step |
|---|---|
| Enter data into template from data report tables | Check 30-50% of hand-entered data and 100% if errors found; ~10% of data pull from electronic files |
| | Check samples from report text: correct type (normal, replicate, etc.), correct matrix |
| | Check tests from report text or validation report: correct methods, correct lab matrix, correct basis |
| | Check results from lab report sheets or validation report: correct analytes, detection limits, units |
| Load templates | Check samples match with tests, tests match with results |
| SCRA data reduction[*a] | Check again for correct sample type, matrix, basis, and units |
| | Check for unusual values and qualifiers |

[*a] Performed by Senior Information Manager

# ~~3.0 RI DATA SET~~

~~The data management rules used to refine the SCRA database for purposes of reporting are described in this section.~~

## ~~3.4~~3.1 CALCULATED TOTALS

This section presents the summation rules for the RI data set and baseline risk assessment data sets and highlights where they differ. Calculated totals were created for analytes evaluated on the basis of summed concentrations. Data management rules for all three data sets are summarized in Table A3-2. ~~The calculated totals include the following: total PCB Aroclors, total PCB congeners, total PAH, total low-molecular-weight PAH (LPAH), total high-molecular-weight PAH (HPAH), carcinogenic PAH (cPAH) reported in benzo(a)pyrene equivalents (BaPEq), total DDD, total DDE, total DDT, total DDx, total chlordanes, total endosulfans, total xylenes, total benzene + toluene + ethylbenzene + xylene (BTEX), total fines, TPH, and total PCDD/Fs. All totals were either T or A qualified to indicate that the values were manipulated values (i.e., summed or selected). The A qualifier was used when all of the individual analytes necessary for the total were not available (i.e., a partial sum).~~

### 3.1.1 General Summation Rules

RI data set summation rules are as follows:

- Calculated totals are the sum of all detected concentrations; non-detected concentrations are treated as zero
- If all analytes for a total are not detected, then the highest detection limit is used for the summation.

Baseline risk assessments and the background data set summation rules are as follows:

- Calculated totals are the sum of all detected concentrations, and non-detected results for analytes detected at least once in the risk assessment data set within the Study Area for a given medium are included in the summation at one-half the detection limit
- If none of the analytes are detected for a given sample, but are determined to be present within the Study Area, then the highest detection limit is used for the summation
- Non-detects for analytes never detected within a data set for a given medium are excluded (i.e., treated as zero).

The determination of medium-specific data sets differs between the BHHRA and the BERA based on relevant exposure scenarios. Medium-specific data sets are described in Appendix F (BHHRA) and Appendix G (BERA).

### 3.1.2 Individual Analytes in Calculated Totals

Data sets for the RI and baseline risk assessments included calculated totals for the chemical groups listed in Table A3-3.

Individual analytes included in totals are as follows:

- **Total PCBs**—Sum of PCB Aroclors or PCB congeners. Total PCB Aroclors represent the sum of all reported Aroclors. Total PCB congeners represent the sum of all reported (up to 209) individual congeners. For the RI and BHHRA data sets, total PCB congeners were selected to represent total PCBs when available. If not available, total PCB Aroclors were selected. Total PCB selection in the BERA varied depending on the medium:
  - For all BERA surface sediment samples, the total PCB concentration is represented by total PCB Aroclors.
  - For the BERA tissue data set, the total PCB concentration is represented by total PCB Aroclors for Round 1 samples and total PCB congeners for Round 2 and Round 3 samples. Aroclors were selected over congeners for Round 1 because PCB congener analysis was performed on only a limited number of samples.
  - For the BERA surface water data set, the total PCB concentration is represented by total PCB congeners for all XAD samples and by total PCB Aroclors for locations where only peristaltic samples were collected.
- **Total PCDD/Fs**[2]—Total polychlorinated dibenzo-p-dioxins/furans (PCDD/Fs) reported in the RI are the sum of tetra and higher polychlorinated dioxin and furan homologs: tetrachlorodibenzo-p-dioxins (TCDDs), pentachlorodibenzo-p-dioxins (PeCDDs), hexachlorodibenzo-p-dioxins (HxCDDs), heptachlorodibenzo-p-dioxins (HpCDDs), octachlorodibenzo-p-dioxin (OCDD), tetrachlorodibenzofurans (TCDFs), pentachlorodibenzofurans (PeCDFs), hexachlorodibenzofurans (HxCDFs), heptachlorodibenzofurans (HpCDFs), and octachlorodibenzofuran (OCDF). Total PCDD/Fs for the BERA were calculated from the sum of individual PCDD/F compounds. The BHHRA relies solely on the 2,3,7,8-TCDD TEQ (toxic equivalent).
- **PCB Congener TEQs**—PCB congener TEQs were calculated using the 2005 World Health Organization (WHO) consensus toxic equivalency factor (TEF) values for mammals (Van den Berg et al. 2006). TEQs were calculated as the

[2] The term "PCDD/Fs" is equal in meaning to "dioxins/furans" in the RI.

sum of each congener concentration (or detection limit for non-detects) multiplied by the corresponding TEF value. When all of the congeners were not detected in a given sample, then the reported TEQ value was the highest congener detection limit multiplied times the TEF value.

- **Dioxin and Furan Congener TEQs**—Dioxin and furan TEQs were calculated using the 2005 WHO consensus TEF values for mammals (Van den Berg et al. 2006). TEQs were calculated as the sum of each detected congener concentration multiplied by the corresponding TEF value. When all of the congeners were not detected in a given sample, then the reported TEQ value was the highest congener detection limit multiplied by the TEF value.

| Compound | TEF |
|---|---|
| **Chlorinated dibenzo-p-dioxins** | |
| **2,3,7,8-TCDD** | **1** |
| 1,2,3,7,8-PeCDD | 1 |
| 1,2,3,4,7,8-HxCDD | 0.1 |
| 1,2,3,6,7,8-HxCDD | 0.1 |
| 1,2,3,7,8,9-HxCDD | 0.1 |
| 1,2,3,4,6,7,8-HpCDD | 0.01 |
| OCDD | 0.0003 |
| **Chlorinated dibenzofurans** | |
| 2,3,7,8-TCDF | 0.1 |
| 1,2,3,7,8-PeCDF | 0.03 |
| 2,3,4,7,8-PeCDF | 0.3 |
| 1,2,3,4,7,8-HxCDF | 0.1 |
| 1,2,3,6,7,8-HxCDF | 0.1 |
| 1,2,3,7,8,9-HxCDF | 0.1 |
| 2,3,4,6,7,8-HxCDF | 0.1 |
| 1,2,3,4,6,7,8-HpCDF | 0.01 |
| 1,2,3,4,7,8,9-HpCDF | 0.01 |
| OCDF | 0.0003 |
| **Non-ortho substituted PCBs** | |
| PCB 77 | 0.0001 |
| PCB 81 | 0.0003 |
| PCB 126 | 0.1 |
| PCB 169 | 0.03 |
| **Mono-ortho substituted PCBs** | |
| PCB 105 | 0.00003 |
| PCB 114 | 0.00003 |
| PCB 118 | 0.00003 |
| PCB 123 | 0.00003 |
| PCB 156 | 0.00003 |
| PCB 157 | 0.00003 |
| PCB 167 | 0.00003 |
| PCB 189 | 0.00003 |

- **Total DDx**—Total DDx was calculated from the six DDx compounds: 2,4′-dichloro-diphenyl-dichloroethane (DDD); 4,4′-DDD; 2,4′-dichloro-diphenyl-dichloroethene (DDE); 4,4′-DDE; 2,4′-dichloro-diphenyl-trichloroethane (DDT); and 4,4′-DDT. Total DDD was calculated with 2,4′-DDD and 4,4′-DDD; total DDE was calculated with 2,4′-DDE and 4,4′-DDE; and total DDT was calculated with 2,4′-DDT and 4,4′-DDT.
- **Total LPAHs**—Total low molecular weight polycyclic aromatic hydrocarbons (LPAHs) are the sum of 2-methylnaphthalene, acenaphthene, acenaphthylene, anthracene, fluorene, naphthalene, and phenanthrene.
- **Total HPAHs**—Total high molecular weight polycyclic aromatic hydrocarbons (HPAHs) are the sum of fluoranthene, pyrene, benzo(a)anthracene, chrysene, benzofluoranthene, benzo(a)pyrene, indeno(1,2,3,-c,d)pyrene, dibenzo(a,h)anthracene, and benzo(g,h,i)perylene.
- **Total PAHs**—Total polycyclic aromatic hydrocarbons (PAHs) are the sum of the individual LPAHs and HPAHs.
- **Total cPAHs**—A benzo(a)pyrene (BaP) equivalent (BaPEq) concentration was calculated by multiplying the carcinogenic PAHs (cPAHs) by their respective potency equivalency factors (PEFs), and summing the resulting concentrations. PAHs classified as carcinogenic are benzo(a)anthracene, chrysene, benzo(b)fluoranthene, benzo(k)fluoranthene, benzo(a)pyrene, indeno(1,2,3,-c,d)pyrene, and dibenzo(a,h)anthracene. PEFs were assigned according to USEPA (1993):

| Analyte | PEF |
|---|---|
| Benzo(a)anthracene | 0.1 |
| Benzo(a)pyrene | 1 |
| Benzo(b)fluoranthene | 0.1 |
| Benzo(k)fluoranthene | 0.01 |
| Chrysene | 0.001 |
| Dibenzo(a,h)anthracene | 1 |
| Indeno(1,2,3-cd)pyrene | 0.1 |

- **Total Chlordanes—**Sum of *cis*-chlordane, *trans*-chlordane, oxychlordane, *cis*-nonachlor, and *trans*-nonachlor.
- **Total Endosulfan**—Sum of alpha-endosulfan, beta-endosulfan, and endosulfan sulfate.
- **Total Xylene**—Sum of *m*,*p*-xylene, *o*-xylene, and xylene.
- **BTEX**—Sum of benzene, toluene, ethylbenzene, and total xylenes.
- **Total Fines**—Sum of all silt and clay grain-size fractions passing U.S. standard sieve #230 (0.0625-mm openings).

- **TPH**—Total petroleum hydrocarbons (TPH) are the sum of diesel-range hydrocarbons, residual-range hydrocarbons, gasoline-range hydrocarbons, lube oil, and motor oil.

For both the RI and baseline risk assessment data sets, a minimum number of individual analytes for a given sample was required to be analyzed in order to complete the totals. These rules are provided in Table A3-4. Totals with less than the expected number of analytes but above the minimum number of analytes were ~~qualified~~identified with ~~an~~the descriptor "A." For PCB and dioxin TEQs, all analytes with TEFs were required in order to calculate a total. Refer to Appendix D for all of the individual values and analytes that were used for the totals in each sample.

~~Summation Rules~~

~~Calculated totals are the sum of all detected concentrations. If all of the analytes were not detected, then the highest reporting detection limit was the selected value for the calculated total, and a U qualifier was added to indicate the lack of detected values.~~

~~The number of analytes required for the calculation of each sum is summarized below. If a limited number of analytes was available, the sum was calculated and A qualified to indicate that not all the expected analytes were available to sum. If an unacceptable number of analytes was available, then the sum was not calculated. For PCB and dioxin TEQs, all analytes with TEFs were required in order to calculate a total. Refer to Appendix D for all of the individual values and analytes that were used for the totals in each sample.~~

| ~~Chemical Name~~ | ~~Expected Analytes~~ | ~~'A' qualify (Limited)~~ | ~~Do Not Sum~~ |
|---|---|---|---|
| ~~Total PCBs-Aroclors (calc'd)~~ | ~~7 or 9~~ | ~~<7~~ | ~~<2~~ |
| ~~Total PCDD/Fs (calc'd)~~ | ~~17~~ | ~~<17~~ | ~~<10~~ |
| ~~Total HPAHs (calc'd)~~ | ~~10~~ | ~~<10~~ | ~~<5~~ |
| ~~Total LPAHs (calc'd)~~ | ~~7~~ | ~~<7~~ | ~~<3~~ |
| ~~Total PAHs (calc'd)~~ | ~~17~~ | ~~<17~~ | ~~<10~~ |
| ~~Total PCB Congeners (calc'd)~~ | ~~209~~ | ~~<150~~ | ~~<100~~ |
| ~~Sum DDD (calc'd)~~ | ~~2~~ | ~~<2~~ | ~~-~~ |
| ~~Sum DDE (calc'd)~~ | ~~2~~ | ~~<2~~ | ~~-~~ |
| ~~Sum DDT (calc'd)~~ | ~~2~~ | ~~<2~~ | ~~-~~ |
| ~~Total Chlordane (calc'd)~~ | ~~5~~ | ~~<5~~ | ~~-~~ |
| ~~Total DDTs (calc'd)~~ | ~~6~~ | ~~<6~~ | ~~-~~ |
| ~~Total Endosulfan (calc'd)~~ | ~~3~~ | ~~<3~~ | ~~-~~ |
| ~~Total Xylenes (calc'd)~~ | ~~2~~ | ~~<2~~ | ~~-~~ |

## 3.79.0 Calculated Totals

Total PCBs were calculated two ways: as total PCB Aroclors and as total PCB congeners. Total PCB Aroclors represented the sum of Aroclors. Total PCB congeners represented the sum of all reported (up to 209) individual congeners.

Total PCDD/Fs were calculated as the sum of dioxin and furan homologs: tetrachlorodibenzo-p-dioxins, pentachlorodibenzo-p-dioxins, hexachlorodibenzo-p-dioxins, heptachlorodibenzo-p-dioxins, octachlorodibenzo-p-dioxin, tetrachlorodibenzofurans, pentachlorodibenzofurans, hexachlorodibenzofurans, heptachlorodibenzofurans, and octachlorodibenzofuran.

Total LPAHs were calculated with the concentrations for 2-methylnaphthalene, acenaphthene, acenaphthylene, anthracene, fluorene, naphthalene, and phenanthrene.

Total HPAHs were calculated with the concentrations for fluoranthene, pyrene, benzo(a)anthracene, chrysene, benzofluoranthenes, benzo(a)pyrene, indeno(1,2,3,-c,d)pyrene, dibenzo(a,h)anthracene, and benzo(g,h,i)perylene.

Total PAHs were calculated with the concentrations of the individual LPAHs and HPAHs.

Total Carcinogenic PAHs (cPAHs) were calculated as follows. A benzo(a)pyrene equivalent (BaPEq) concentration was calculated by multiplying the carcinogenic PAHs by their respective potency equivalent factors (PEFs), and summing the resulting concentrations. PAHs classified as carcinogenic are benzo(a)anthracene, benzo(a)pyrene, benzo(b)fluoranthene, benzo(k)fluoranthene, chrysene, dibenzo(a,h)anthracene, and indeno(1,2,3,-c,d)pyrene. PEFs were assigned according to EPA (1993):

| Analyte | PEF |
|---|---|
| Benzo(a)anthracene | 0.1 |
| Benzo(a)pyrene | 1 |
| Benzo(b)fluoranthene | 0.1 |
| Benzo(k)fluoranthene | 0.01 |
| Chrysene | 0.001 |
| Dibenzo(a,h)anthracene | 1 |
| Indeno(1,2,3-cd)pyrene | 0.1 |

Total DDx were calculated with the concentrations of the six DDx compounds: 2,4′-DDD; 4,4′-DDD; 2,4′-DDE; 4,4′-DDE; 2,4′-DDT; and 4,4′-DDT. Total DDD were calculated with 2,4′-DDD and 4,4′-DDD; total DDE were calculated with 2,4′-DDE and 4,4′-DDE; and total DDT were calculated with 2,4′-DDT and 4,4′-DDT.

Total LPAHs were calculated with the concentrations for 2-methylnaphthalene, acenaphthene, acenaphthylene, anthracene, fluorene, naphthalene, and phenanthrene. Total HPAHs were calculated with the concentrations for fluoranthene, pyrene,

benzo(a)anthracene, chrysene, benzofluoranthenes, benzo(a)pyrene, indeno(1,2,3, c,d)pyrene, dibenzo(a,h)anthracene, and benzo(g,h,i)perylene. Total PAHs were calculated with the concentrations of the individual LPAHs and HPAHs. Total Carcinogenic PAHs (cPAHs) were calculated with the concentrations for benzo(a)anthracene, chrysene, benzofluoranthenes, benzo(a)pyrene, indeno(1,2,3, c,d)pyrene, and dibenzo(a,h)anthracene.

Total chlordanes were calculated as the sum of the following compounds: cis-chlordane, trans-chlordane, oxychlordane, cis-nonachlor, and trans-nonachlor.

Total endosulfans were calculated as the sum of alpha-endosulfan, beta-endosulfan, and endosulfan sulfate.

Total xylenes were calculated as the sum of m,p-xylene and o-xylene.

BTEX were calculated as the sum of benzene, toluene, ethylbenzene, and xylenes.

Total fines were calculated as the sum of all silt and clay grain-size fractions passing U.S. standard sieve #230 (0.0625-mm openings).

Total petroleum hydrocarbons were calculated as the sum of diesel-range hydrocarbons, residual-range hydrocarbons, gasoline-range hydrocarbons, lube oil, and motor oil.

## 3.119 CALCULATION OF TOXICITY EQUIVALENTS

### 3.120.0 Calculation of PCB Congener TEQs

PCB congener toxic equivalents (TEQs) were calculated using the 2005 World Health Organization (WHO) consensus toxic equivalency factor (TEF) values for mammals (Van den Berg et al. 2006). TEQs were calculated as the sum of each congener concentration (or detection limit for non-detects) multiplied by the corresponding TEF value. When all of the congeners were not detected in a given sample, then the reported TEQ value was the highest congener detection limit multiplied times the TEF value.

### 3.122.0 Calculation of Dioxin and Furan TEQs

Dioxin and furan TEQs were calculated using the 2005 WHO consensus TEF values for mammals (Van den Berg et al. 2006). TEQs were calculated as the sum of each detected congener concentration multiplied by the corresponding TEF value. When all of the congeners were not detected in a given sample, then the reported TEQ value was the highest congener detection limit multiplied by the TEF value.

| Compound | TEF |
|---|---|
| **Chlorinated dibenzo-p-dioxins** | - |
| 1,2,3,7,8-PeCDD | 1 |
| 1,2,3,4,7,8-HxCDD | 0.1 |
| 1,2,3,6,7,8-HxCDD | 0.1 |

| Compound | TEF |
|---|---|
| 1,2,3,7,8,9-HxCDD | 0.1 |
| 1,2,3,4,6,7,8-HpCDD | 0.01 |
| OCDD | 0.0003 |
| **Chlorinated dibenzofurans** | |
| 2,3,7,8-TCDF | 0.1 |
| 1,2,3,7,8-PeCDF | 0.03 |
| 2,3,4,7,8-PeCDF | 0.3 |
| 1,2,3,4,7,8-HxCDF | 0.1 |
| 1,2,3,6,7,8-HxCDF | 0.1 |
| 1,2,3,7,8,9-HxCDF | 0.1 |
| 2,3,4,6,7,8-HxCDF | 0.1 |
| 1,2,3,4,6,7,8-HpCDF | 0.01 |
| 1,2,3,4,7,8,9-HpCDF | 0.01 |
| OCDF | 0.0003 |
| **Non-ortho substituted PCBs** | |
| PCB 77 | 0.0001 |
| PCB 81 | 0.0003 |
| PCB 126 | 0.1 |
| PCB 169 | 0.03 |
| **Mono-ortho substituted PCBs** | |
| PCB 105 | 0.00003 |
| PCB 114 | 0.00003 |
| PCB 118 | 0.00003 |
| PCB 123 | 0.00003 |
| PCB 156 | 0.00003 |
| PCB 157 | 0.00003 |
| PCB 167 | 0.00003 |
| PCB 189 | 0.00003 |

## 3.2 FIELD REPLICATES

For the RI, the BHHRA, and the BERA data sets, field replicates were generally retained as individual sample results. For spatial analyses requiring the calculation of spatially weighted average concentrations, only one sample result was used for those results with identical sampling coordinates. In those cases, data associated with the first sample were used in the analysis. Field replicates in the background data set were averaged to avoid bias by overweighing a single sample location. The potential for bias is greater in the background data set due to the small number of samples. Otherwise, data presentations and analyses included field replicates as discrete samples.

## 3.3 ORGANIC CARBON NORMALIZATION

Organic chemical results were organic carbon normalized (OC normalized) for subsequent evaluation in the BERA and background data sets, following the criteria described in Table A3-2. Dry-weight concentrations in mg/kg were divided by the decimal percent total organic carbon (TOC) value.

No upper TOC limit was set that would exclude normalization; however, for higher TOC values (>4.0%), each individual sample was evaluated for possible anthropogenic contributions to organic carbon (e.g., wood waste, petroleum, nonaqueous--phase liquids [NAPLs], or sewage) that may have confounded partitioning assumptions. For TOC <0.2%, or high values with contribution from anthropogenic wastes, no OC-normalized value was calculated. In these few cases, sample data were evaluated on a dry-weight basis only. For samples without TOC data, the value was estimated using a regression equation based on site-specific TOC and grain size (as percent fines) from the upriver reach (RM >15.3).

### ~~3.223~~3.4 SIGNIFICANT FIGURES

The laboratories provided results in electronic text files. The text values were maintained in the database so that the number of significant figures provided by the labs would not be lost by either the addition or removal of trailing zeros. For example, if the lab file contained 1.0, then that text string would be maintained to avoid conversion to either 1.00 or 1. In some cases, the lab reported value appeared to have only one significant figure (1, for example). But a minimum of two significant figures was assumed for all results, which was consistent with the standard reporting requirements of analytical laboratories.

During calculations, such as averaging replicates or summing for totals, all significant figures were carried through the calculation. The final result was then rounded to the smallest number of significant figures found in the values used in the calculation. For example: 7010 + 105 + 20.8 = 7135.8, and with three significant figures equals 7140.

## 4.0 RI DATA SET

The data set used for each RI data type is summarized in Table A3-5. The first column of the table lists the various data types. The second column lists the data sources and the general data quality selection criteria (e.g., Category 1 versus Category 2 and QA1 versus QA2). Additional data inclusion or exclusion criteria used for subsequent data analyses and presentations in the RI report are listed in the third column. Further data evaluation steps, such as the outlier analysis, that are specific to a particular data set, are not included here but are discussed in the appropriate RI report sections. A complete list of data exclusions for each data type is provided in Appendix A2. The RI data set is provided electronically as a CD attachment to this appendix.

## 5.0 BHHRA DATA SET

The data set used for each BHHRA data type is summarized in Table A3-6. The first column of the table lists the various data types. The second column lists the data sources and the general data quality selection criteria (e.g., Category 1 vs. Category 2 and QA1 vs. QA2). Additional data inclusion or exclusion criteria used to develop the BHHRA data set are listed in the third column. Specific data management procedures

and rules and additional data reduction steps for the BHHRA are provided in Appendix F.

## 6.0 BERA DATA SET

The data set used for each BERA data type is summarized in Table A3-7. Taken together, the inclusion and exclusion criteria listed below were used to develop the BERA data set. Specific data management procedures and rules and additional data reduction steps for the BERA are provided in Appendix G.

## 7.0 QUERY MANAGER™ DATABASE

USEPA and its government partners, as well as members of the general public, use the Query Manager™ database-mapping application developed by the National Oceanic and Atmospheric Administration's (NOAA) National Ocean Service Office of Response and Restoration.[3] Sediment and biota chemistry data contained in the SCRA database were translated into Query Manager-compatible format files and uploaded to NOAA's Portland Harbor Watershed Database. Currently, water data are not stored in Query Manager. NOAA has integrated the Portland Harbor Watershed Database with data query software (MARPLOT®) and ArcView® GIS on a web-based portal (http://mapping2.orr.noaa.gov/website/portal/portland/). Users may analyze and display the data contained in Query Manager along with spatial information, such as aerial photos, bathymetry, shoreline types, and outfalls.

Summing methods used in Query Manager for the various compound groups discussed above depart slightly from the LWG's summing methods. In all cases, non-detects for individual substances in a compound group are treated as zero values, and if the sum of detected results for individual substances in a sample is less than the maximum non-detected result, then the sum is reported at the higher detection limit with a U-qualifier. Specific summing rules are provided below:

- **Total PCBs**—Aroclor and congener data are summed separately (PCB SUM A [total Aroclors] and PCB SUM P [total congeners]). In Query Manager, the preferred PCB sum is reported for the Aroclor data since those data are reported for the majority of studies. In the LWG database, the preferred PCB sum is reported for the congener data.
- **Total DDx**—Calculated using six isomers where available. If three or fewer isomers are reported, the sums are not derived (routine assumes that only p,p'-isomers were reported). Also, the sum of isomer pairs of DDT and its derivatives were calculated. The following pairs were summed when both isomers were provided for samples in the data set: 2,4'-DDT and 4,4'-DDT; 2,4'-DDD and 4,4'-DDD; 2,4'-DDE and 4,4'-DDE.

[3] The LWG relies on the Portland Harbor SCRA database for decision-making purposes and reporting.

- **Total LPAHs**—Sum of acenaphthene, anthracene, biphenyl, 2,6-dimethylnaphthalene, fluorene, 1-methylnaphthene, 2-methylnapthene, 1-methylphenanthrene, phenanthrene, naphthalene, where two or more are measured.
- **Total HPAHs**—Sum of benzo(a)anthracene, benzo(a)pyrene, benzo(e)pyrene, chrysene, dibenzo(a,h)anthracene, fluoranthene, perylene, and pyrene, where two or more are measured.
- **Total PAHs**—Calculated as the sum of the LPAH and HPAH chemicals. Only those samples with more than one chemical in the group (LPAH and HPAH) are summed.
- **Total Chlordanes**—Sum of alpha-chlordane, gamma-chlordane, beta-chlordane, cis- and trans-chlordane, oxychlordane, cis-nonachlor, and trans-nonachlor.

All field duplicates and splits are retained in the Query Manager database and are recorded as separate samples reported from the same location and similar species/tissue type (if applicable) or depths. No data within the Query Manager database is an average. For some queries run with the Query Manager interface, if there are two results with the same StationID/SampleID (lab replicates), the result that has been designated as the preferred result (the "normal" sample) is reported in the queries. "Multi-chem" queries show both the main sample results and lab replicate results.

To illustrate the outcome of a query first performed on the RI data set and then performed in Query Manager, the following example is provided. Table column headings below are those provided in the respective data sets and offer corresponding information. In this example, total LPAHs were queried for samples collected from a surface sediment location (DG-11) in Round 3. Field splits (DG11-2 and DG11-3) were also collected from this location.

From Query Manager:

| Stationid | exsampid | chemcode | conc | qualcode | units |
|---|---|---|---|---|---|
| DG11-1 | LW3-DG11 | LPAH | 30.1 | CALC | PPB |
| DG11-2 | LW3-DG11-2 | LPAH | 142.9 | CALC | PPB |
| DG11-2 | LW3-DG11-3 | LPAH | 155.7 | CALC | PPB |

From RI Data Set:

| LocationName | SampleID | cas_rn | ValueNum | Qualifiers | Units |
|---|---|---|---|---|---|
| DG11-1 | LW3-DG11 | LPAH | 32 | JT | ug/kg |
| DG11-2 | LW3-DG11-2 | LPAH | 160 | JT | ug/kg |

Because no field splits are averaged in Query Manager, three separate total LPAH results were reported. Further, because total LPAHs are calculated using an analyte list

that differs from the RI data set, and because splits are averaged in the RI data set, the calculated totals are different. In this case, the results reported in the RI data set are slightly higher than the results reported in Query Manager.

## 4.0 QUALIFIER DEFINITIONS

The following qualifier definitions are applied to data contained in the SCRA database.

| Qualifier | Description |
|---|---|
| A | Summed value based on limited number of analytes. |
| J | Estimated value. |
| JA | Combined qualifier. |
| JT | Combined qualifier. |
| N | Presumptive evidence of a compound. |
| NJ | Combined qualifier. |
| NJT | Combined qualifier. |
| NT | Combined qualifier. |
| R | Rejected. |
| T | Result derived or selected from >1 reported value. |
| U | Analyte was analyzed for but not detected. |
| UA | Combined qualifier. |
| UJ | Not detected. Sample detection limit is estimated. |
| UJA | Combined qualifier. |
| UJT | Combined qualifier. |
| UT | Combined qualifier. |

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